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Modeling Partially-Collisional Plasmas using Finite-size Particles with Internal Dynamics

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Modeling Partially-Collisional Plasmas using Finite-size Particles with Internal Dynamics*

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We report recent results from our effort to develop "smart" particle methods. Unlike traditional PIC particles, the CPK (Complex Particle Kinetics) algorithm [1] allows particles with a Gaussian spatial profile and a Mawellian velocity distribution to evolve self-consistently. These particles are then split spatially and/or in velocity to probe for emerging features as the simulation progresses. Aggressive merging is employed to control the number of simulation particles. An algorithm for modeling collisional plasmas using point particles with Maxwellian velocity distributions has been developed and reproduces known Monte-Carlo PIC results with less noise and significantly fewer particles[2]. The combination of the CPK algorithm with our new collision algorithm should allow simulation of plasmas in the previously cost-prohibitive partially-collisional regime. Results from one-dimensional simulations will be compared to experimental data and 2 and 3-D results will be discussed.

Evolution equations

Unlike the traditional PIC technique we make use of particle with finite spatial extent and finite temperature. The spatial profile is taken to be a Gaussian, which facilitates splitting and merging, and the velocity distribution is assumed to be Maxwellian, allowing the use of well-known collisional frequencies. The particles have the following description [1] in (x,t) space:

$$f_o(x,t) = \frac{W_o}{\sqrt{2\pi}\, w_{do} v_{to}} e^{-\frac{\{x-x_o-(v-v_o)t\}^2 k}{2w_{do}^2} - \frac{(v-v_o)^2}{2v_{to}^2}} \tag{1}$$

The particle can also be represented by the equivalent expression in (x,R) space:

$$f_o(x,R) = \frac{W_o}{\sqrt{2\pi}\, w_{do} v_{to}} e^{-\frac{(x-x_0)^2}{2w_{do}^2} - \frac{(v-v_o-R(x-x_0))^2}{2v_{to}^2}} \tag{2}$$

Individual particle evolution is accomplished via the collisionless expansion equations:

$$\begin{aligned} V_{t0}^2 &= \frac{w_{d0}^2 v_{t0}^2}{w_{d0}^2 + v_{t0}^2 t^2}; \\ R &= \frac{v_{t0}^2 t}{w_{d0}^2 + v_{t0}^2 t^2} \\ W_{d0}^2 &= w_{d0}^2 + v_{t0}^2 t^2 \end{aligned} \tag{3}$$

Splitting procedure

As the particles evolve, they are continually split into smaller particles, either in x or v space. This allows the particles to "probe" the simulation space for emerging features. Merging particles is essential to control the particle number and our current procedure is explained in the following section. We can split the particles in either space using a procedure the preserves the first four moments of the x or v distribution exactly. The following example is for velocity space splitting and comprises the 0th, 2nd, and 4th moments:

$$w_0 = w_m + 2w_p \tag{4}$$

$$\begin{aligned}\left(u_{x0}^2 + v_{thx0}^2 + v_{thy0}^2 + v_{thz0}^2\right)w_0 &= \left(u_{x0}^2 + v_{thxm}^2 + v_{thy0}^2 + v_{thz0}^2\right)w_m + \\ &\left(\left(u_{x0} - u_{xp}\right)^2 + v_{thxp}^2 + v_{thy0}^2 + v_{thz0}^2\right)w_p + \left(\left(u_{x0} + u_{xp}\right)^2 + v_{thxp}^2 + v_{thy0}^2 + v_{thz0}^2\right)w_p\end{aligned} \tag{5}$$

$$\begin{aligned}\left(u_{x0}^4 + 2v_{thx0}^2v_{thy0}^2 + 2v_{thx0}^2v_{thz0}^2 + 3v_{thx0}^4 + 2u_{x0}^2\left(3v_{thx0}^2 + v_{thy0}^2 + v_{thz0}^2\right)\right)w_0 &= \\ \left(u_{x0}^4 + 2v_{thxm}^2v_{thy0}^2 + 2v_{thxm}^2v_{thz0}^2 + 3v_{thxm}^4 + 2u_{x0}^2\left(3v_{thxm}^2 + v_{thy0}^2 + v_{thz0}^2\right)\right)w_m + \\ \left(\left(u_{x0} - u_{xp}\right)^4 + 2v_{thxp}^2v_{thy0}^2 + 2v_{thxp}^2v_{thz0}^2 + 3v_{thxp}^4 + 2\left(u_{x0} - u_{xp}\right)^2\left(3v_{thxp}^2 + v_{thy0}^2 + v_{thz0}^2\right)\right)w_p + \\ \left(\left(u_{x0} + u_{xp}\right)^4 + 2v_{thxp}^2v_{thy0}^2 + 2v_{thxp}^2v_{thz0}^2 + 3v_{thxp}^4 + 2\left(u_{x0} + u_{xp}\right)^2\left(3v_{thxp}^2 + v_{thy0}^2 + v_{thz0}^2\right)\right)w_p\end{aligned} \tag{6}$$

with the original particle (quantities denoted by the zero subscript) split into three new particles. We assume that the middle particle, denoted subscript *m*, has the same drift velocity as the original particle. If we assume some relationship between w_m and w_p we can solve for v_{thxm} and v_{thxp} in terms of v_{thx0} and u_{xp}. If we choose $w_m = 4w_p$, one of the possible solutions is:

$$v_{thxm} = \sqrt{3v_{thx0}^2 - u_{xp}^2}\Big/\sqrt{3}, \quad v_{thxp} = \sqrt{3v_{thx0}^2 - u_{xp}^2}\Big/\sqrt{3} \tag{7}$$

Equation (7) requires $u_{xp} < \sqrt{3}v_{thx0}$ and produces middle and probe particles with the same thermal velocity.

The choice of u_{xp} must be made with some care as it is possible to satisfy Eqs. (4-6) and significantly alter the shape of the velocity distribution. Very good agreement is achieved with $u_{xp} = 0.5v_{thx0}$; we typically run with $u_{xp} = v_{thx0}$.

Merging technique

Simulation particles are merged in order to reduce the number of active particles and increase computational efficiency. Local average distributions in x and v space are constructed using all the particles local to a specified point. Then individual particles are compared to the local average distribution to determine if they are subsumed by the average distribution. If so, then the particle is merged. Successive particles are added to the emerging distribution and the sum then becomes a new particle. The particles contributing to the sum are then deleted. In practice this procedure works fairly well, although we have seen the results of overly aggressive merging in simulations of two colliding plasma beams.

Collision algorithm

Collisions are modeled by pairing particles. The collisions are weighted using a modified form of the Miller-Combi collision algorithm [3], which allows a reduced number of pairings per time-step compared to the traditional Takizuka and Abe [4] approach. The simulation particle velocities and temperatures are adjusted using the collision frequencies for colliding Maxwellians. The density, temperature, and mass of species α are n_α, T_α, and m_α. The reduced mass is $m_{\alpha\beta} = m_\alpha m_\beta / (m_\alpha + m_\beta)$. The two collision frequencies, $\nu_{\alpha\beta}$ and $\nu^{\varepsilon}_{\alpha\beta}$, are given by

$$\nu_{\alpha\beta} = \frac{8\sqrt{\pi} Z_\alpha^2 Z_\beta^2 e^4 n_\beta \ln\Lambda_{\alpha\beta}}{m_{\alpha\beta}^2 (\Delta v)^3}\left[\frac{\sqrt{\pi}}{2}\mathrm{erf}\left(\frac{\Delta v}{v_{th}}\right) - \left(\frac{\Delta v}{v_{th}}\right)\exp\left(-\frac{\Delta v^2}{v_{th}^2}\right)\right] \tag{8}$$

and

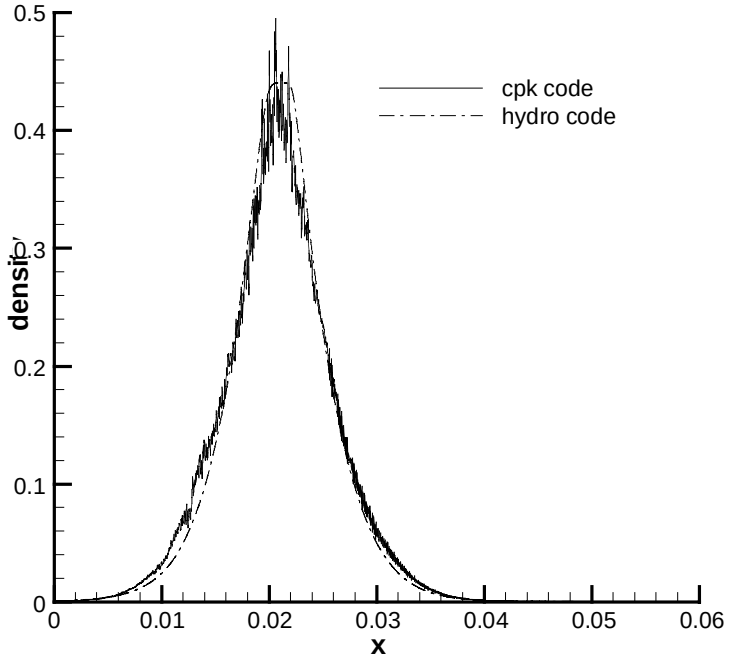
$$\nu^{\varepsilon}_{\alpha\beta} = \frac{16\sqrt{\pi} Z_\alpha^2 Z_\beta^2 e^4 n_\beta \ln\Lambda_{\alpha\beta}}{m_\alpha m_\beta v_{th}^3}\exp\left(-\frac{\Delta v^2}{v_{th}^2}\right) \tag{9}$$

where $v_{th}^2 \equiv 2k_B(T_\alpha/m_\alpha + T_\beta/m_\beta)$, $\Delta v \equiv \left|\vec{v}_\alpha - \vec{v}_\beta\right|$, $\ln\Lambda_{\alpha\beta}$ is the Coulomb logarithm, and $Z_\alpha e$ is the charge of species α. Jones *et.al*. [5] identify the frequency given by Eq. (8) with dynamic friction, while that given by Eq.(9) is related to temperature equilibration.

Collisional to collisionless example

The collisional model and internal dynamics described above have been implemented in one and two dimensional codes in a hybrid scheme using the quasi-neutral assumption. Here we show some results from a 1-D simulation of an experiment consisting of solid slab of aluminum ionized by a laser and traveling to the right with a velocity of 2×10^6 cm/s. The slab is highly collisional at the start of the simulation with a solid density, 2.21×10^{22} particles per cc, and low temperature $T_i = T_e = 5.56$ eV. The slab expands at the ion sound speed until the leading edge becomes non-collisional. The plasma collides with another slab of material at the right end of the simulation and the

pressure is measure here as a function of time. Simulations of this experiment using a fluid code show a pressure vs time curve that comes up late in time and too sharply compared to the experimental data. Our result shows a softer ramp-up in pressure starting at an earlier time. The figure below shows the simulation particle phase space. The particle size is proportional to the weight of the simulation particles.



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